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ON ZAGREB COINDEX POLYNOMIALS FOR SOME SPECIAL GRAPHS

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Abstract. Zagreb polynomial is a polynomial in which the power of the indeterminate is a Zagreb index, Zagreb index is a graph invariant as it remains fixed under graph homomorphism. The complement of a graph is needed to compute the Zagreb coindex as well as the polynomial. In this paper we looked at the size of the complement graphs under consideration and the formulae for their Zagreb coindex polynomials.The graphs are cycle C_n, wheel W_n, path P_n, complete graph K_n and the complete bipartite graph $K_{m,n}$.

1. Introduction

Topological indicies are values obtained from graphs, they are also called graph invariants as they remain fixed under graph homomorphism [5] and as stated in [9] the significance of topological indicies lies in their ability to transform complex molecular structures into numerical representations which is done via the use of graphs and this helps in building computational models used in different fields like drug discovery, material science and reaction chemistry. Graph $\Gamma(V, E)$ [3] is an ordered pair consisting of set of vertices V and set of edges E with elements of E linking elements of V. The order of Γ is given by the cardinality of V while the size is given by E.

A lot of topological indices have been developed either from chemistry or mathematical perspective, just like the first and second Zagreb indices introduced by Gutman and Trinajstic [4] in 1972 which they defined interms of the degree of vertices of a graph. The degree of a vertex v denoted as d_v is the number of edges incident with v [2], i.e the number of edges linking v with other vertices in the graph. The two Zagreb indices are defined as follows; the first

$$M_1(\Gamma) = \sum_{v \in V(\Gamma)} (d_v)^2 \tag{1.1}$$

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and the second is define as

$$M_2(\Gamma) = \sum_{uv\in E(\Gamma)} d_u \ . \ d_v \tag{1.2}$$

Parvez [7] later showed that the first Zagreb index is also written as

$$M_1(\Gamma) = \sum_{uv\in E(\Gamma)} [d_u + d_v] \tag{1.3}$$

and that the redefined third Zagreb index is computed using

$$ReZG_3(\Gamma) = \sum_{uv\in E(\Gamma)} [d_u \ . \ d_v][d_u + d_v] \ . \tag{1.4}$$

There is the Wiener's index [8] which is defined as

$$W(\Gamma) = \frac{1}{2} \sum_{\{u,v\}\subseteq V(\Gamma)} d(u, v) \ , \tag{1.5}$$

it is defined in terms of the distance between two vertices u and v which we denote as $d(u, v)$, where distance in this case refers to the number of few edges between the vertices [2], the distance is by taking the shortest path between the two vertices. The distance between vertices is also used in getting the eccentricity of a vertex. The eccentricity [1] of a vertex v ($ecc(v)$) is the maximum distance between v and a vertex farthest away from it.

There are polynomials associated with topological indices, these are polynomials whose coefficient and power of the indeterminate are topological indices. As can be seen in; the first and second Zagreb polynomials [11] below

$$M_1(\Gamma; x) = \sum_{uv\in E(\Gamma)} x^{d_u+d_v} \tag{1.6}$$

and

$$M_2(\Gamma; x) = \sum_{uv\in E(\Gamma)} x^{d_u \ . \ d_v}. \tag{1.7}$$

The Wiener's polynomial [8] is obtained using

$$W(\Gamma; x) = \frac{1}{2} \sum_{\{u,v\}\subseteq V(\Gamma)} x^{d(u,v)} \tag{1.8}$$

while the eccentric connectivity polynomial [6] is given as

$$ECP(\Gamma; x) = \sum_{v\in V(\Gamma)} d_v x^{ecc(v)} \ . \tag{1.9}$$

2. Result

Doslic [12] introduced the Zagreb Coindices of a graph, the first Zagreb coindex is defined as

$$\bar{M}_1(\Gamma) = \sum_{uv\notin E(\Gamma)} [d_u + d_v] \tag{2.1}$$

while the second Zagreb coindex is defined as

$$\bar{M}_2(\Gamma) = \sum_{uv \notin E(\Gamma)} [d_u \, . \, d_v] \tag{2.2}$$

with u and v distinct. To get the coindex of a graph Γ we need the complements of the graph $(\bar{\Gamma})$ in question. We got motivated by Equations 1.6 to 1.9 as such we define the first and second Zagreb coindex polynomials. In this paper we considered the cycle graph C_n, wheel W_n, path P_n, complete graph K_n and complete bipartite graph $K_{m,n}$.

Definition 2.1. First Zagreb coindex polynomial of a graph Γ is a polynomial whose degree of the indeterminate x is the sum of the degrees of pair of adjacent vertices (u, v) found in the complement of Γ; and this is written as;

$$\bar{M}_1(\Gamma; x) = \sum_{uv \notin E(\Gamma)} x^{[d_u \, + \, d_v]} \tag{2.3}$$

Definition 2.2. Second Zagreb coindex polynomial of a graph Γ is a polynomial whose degree of the indeterminate x is the product of the degrees of pair of adjacent vertices (u, v) found in the complement of Γ; and this is written as;

$$\bar{M}_2(\Gamma; x) = \sum_{uv \notin E(\Gamma)} x^{[d_u \, . \, d_v]} \tag{2.4}$$

2.1. **Coindex Polynomials for cycle graph C_n.**

Remark 2.3. For every vertex $v_i \in V(C_n)$ $d_{v_i} = 2$ [3].

The proposition below gives the size of the complement of C_n.

Proposition 2.4. *The size of the complement graph of a cycle is given by* $|E(\bar{C}_n)| = \frac{n(n-3)}{2}$.

Proof. The degree of vertices of a complement of a graph is with respect to the old graph [13], so $d_{v_i} = 2, \forall \; v_i \in C_n$ as seen in Remark 2.3. Making v_i adjacent to $(n-3)$ vertices in $\bar{C}_n$ leading to $(n-3)$ edges between a vertex v_i and $(n-3)$ vertices. Applying the hand shaking lemma [2] on all the n vertices gives $|E(\bar{C}_n)| = \frac{n(n-3)}{2}$. □

Lemma 2.5. *The first Zagreb coindex for a cycle C_n is given by the expression $2n(n-3)$.*

Proof. From Equation 2.1 it is clear that the defining sum runs over the edge of the complement of the graph in question (C_n) but the degree of the vertices is with respect to the old graph [13], as such $d_{v_i} = 2$ as seen in Remarks 2.3 making v_i to be adjacent to $(n-3)$ vertices in $\bar{C}_n$. So applying handshaking lemma [2] gives $|E(\bar{C}_n)| = \frac{n(n-3)}{2}$.

$$\Rightarrow \bar{M}_1(C_n) = \sum_{uv \notin E(C_n)} [d_u \; + \; d_v] = \frac{n(n-3)}{2} \times 4 = 2n(n-3).$$

□

Theorem 2.6. *The first Zagreb coindex polynomial for a cycle C_n is a monomial of the form $\frac{n(n-3)}{2}x^4$.*

Proof. From the formula for computing the first Zagreb coindex polynomial the power is gotten by adding the degrees of pair of adjacent vertices . This implies that the coefficient is the size of the graph C_n. □

Since all vertices of C_n are of equal degrees note that

$$\bar{M}_1(C_n) = \sum_{uv \notin E(C_n)} [d_u \ + \ d_v] = \sum_{uv \notin E(C_n)} [d_u \ . \ d_v] \ = \bar{M}_2(\Gamma)$$

which means their Zagreb coindex polynomials are the same.

2.2. **Coindex Polynomials for wheel graph W_n.** Note that a wheel is derived from a cycle C_{n-1} by adding a single vertex K_1 [2] in such a way that the added vertex is adjacent to all the $n-1$ vertices; $W_n = C_{n-1} + K_1$. The size of a wheel is given by $2(n-1)$ [3] and the order is n.

Remark 2.7. The degree of each $v_i \in V(C_{n-1})$ is 3 while that of K_1 is $(n-1)$ [3].

Proposition 2.8. *The Zagreb coindex of a wheel graph W_n is equivalent to the coindex of a cycle graph C_{n-1} which leads to the wheel graph.*

Proof. To get the coindex of a graph Γ we need to get the degree sum of vertices forming an edge in the compliment of $(\bar{\Gamma})$, i.e vertices not adjacent in Γ. So in this case it suffices to show that the size of $\bar{C}_{n-1}$ equals the size of $\bar{W}_n$.
Observe that the added vertex K_1 in W_n is adjacent to all vertices as such not adjacent to any vertex in $\bar{W}_n$ leaving only vertices of C_{n-1} adjacent in the compliment which indicates size of $\bar{W}_n = \bar{C}_{n-1}$. □

Note that the coindex polynomials for $\bar{C}_{n-1}$ and $\bar{W}_n$ are equal.

2.3. **Coindex Polynomials for graph P_n.** The order of a path graph P_n is n while the size is $(n-1)$ [1].

Remark 2.9. In P_n there are 2 edges linking end vertices each of degree 1 to vertices of degree 2 while the remaining $(n-3)$ edges link vertices of degrees 2 [1].

For the coindex of a path graph we need to get the size of the complement graph of a path graph, the proposition below gives the size.

Proposition 2.10. *For a path $P_n (n > 2)$ the size of the complement graph $|E(\bar{P}_n)| = \frac{(n-1)(n-2)}{2}$.*

Proof. The two end vertices are of degree 1 so each is adjacent to $(n-2)$ vertices in $\bar{P}_n$ leading to $(n-2)$ edges while the remaining $(n-2)$ vertices each is adjacent to $(n-3)$ in $\bar{P}_n$ leading to $(n-3)$ edges. So adding all the edges and applying the hand shaking lemma will give;
$|E(\bar{P}_n)| = \frac{2(n-2)+(n-2)(n-3)}{2} = \frac{(n-2)(n-1)}{2}$. □

Example 2.11. Given a path graph P_5 with vertex set $V = \{a, b, c, d, e\}$ and edge set $\{e_1, e_2, e_3, e_4\}$ where $e_1 = \{a, b\}$, $e_2 = \{b, c\}$, $e_3 = \{c, d\}$ and $e_4 = \{d, e\}$. Clearly a is not adjacent to vertices $\{c, d, e\}$, b is not adjacent to vertices $\{d, e\}$ and c is not adjacent to vertex e. The non-adjacent vertices will now be adjacent in the complement. So the complement $\bar{P}_5$ is of size 6 with the following edges $e_1 = \{a, c\}, e_2 = \{a, d\}, e_3 = \{a, e\}, e_4 = \{b, d\}, e_5 = \{b, e\}, e_6 = \{c, e\}$.

The number of edges (size) can be confirmed using Proposition 2.10 as shown below

$|E(\bar{P}_5)| = \frac{(n-2)(n-1)}{2} = \frac{(5-2)(5-1)}{2} = \frac{12}{2} = 6.$

Lemma 2.12. *The first Zagreb coindex for a path graph is given by* $2n^2 - 8n + 8$.

Proof. The end vertices v_1 and v_n of a path graph P_n are each of degree 1 and the two will now be adjacent in $\bar{P}_n$ linked by a single edge. And each vertex will be adjacent to $(n-2)$ vertices in the new graph (i.e excluding itself and the vertex adjacent to it in P_n) meaning there are $2(n-2)$ edges between v_1, v_n and other vertices leading to

$$2(n-2) - 1 = (2n-5) \text{ } edges \tag{1}$$

since the edge linking the end-vertices was counted twice. For the remaining $(n-2)$ vertices which are all of degree 2 the number of edges between them will be

$$|E(\bar{P}_n)| - (2n-5) = \frac{(n-1)(n-2)}{2} - (2n-5) = \frac{n^2 - 7n + 12}{2} \text{ } edges \tag{2}$$

Note that pairing two vertices each of degree 2 gives the sum of degrees as 4 and 3 if one is an end vertex, while for the single edge connecting the end vertices we get sum of degree as 2. So applying (1) and (2) to Equation 2.1 will produce

$$\bar{M}_1(P_n) = \sum_{uv \notin E(P_n)} [d_u + d_v] = 3(2n-6) + 2 \times 1 + 4\frac{(n^2 - 7n + 12)}{2} = 2n^2 - 8n + 8.$$

□

Theorem 2.13. *The first Zagreb coindex polynomial for a path is given by* $x^2 + (2n-6)x^3 + \frac{n^2-7n+12}{2}x^4$.

Proof. The polynomial has coefficients as the number of edges linking vertices that gives a particular sum of degrees, as shown in proof of Lemma 2.12 a single edge link vertices whose degree sum is 2, $(2n-6)$ edges link vertices whose sum of degrees is 3 and $\frac{n^2-7n+12}{2}$ edges link vertices with degree sum as 4. We then use Equation 2.3 to get the polynomial

$$\bar{M}_1(P_n; x) = \sum_{uv \notin E(P_n)} x^{[d_u \, + \, d_v]} = x^2 + (2n-6)x^3 + \frac{n^2 - 7n + 12}{2}x^4.$$

□

Lemma 2.14. *The second Zagreb coindex for a path graph* P_n *is* $2n^2 - 10n + 13$.

Proof. To get the second Zagreb coindex we need the product of degree of vertices making an edge in $\bar{P}_n$, recall from the proof of Lemma 2.12 that we have 1 common edge between v_1 and v_n which gives product of degrees as 1, we have $(2n-6)$ edges linking an end-vertex and other vertices leading to a product of degrees as 2 and the remaining $\frac{n^2-7n+12}{2}$ edges each has vertices whose product of degrees is 4. We then apply Equation 2.2

$$\bar{M}_2(P_n) = \sum_{uv \notin E(P_n)} [d_u \ . \ d_v] = 1 + 2(2n-6) + \frac{n^2-7n+12}{2} \times 4$$
$$= 1 + 2(2n-6) + 2(n^2-7n+12) = 2n^2 - 10n + 13.$$

□

Theorem 2.15. *The second Zagreb polynomial for a path graph is given by* $x + (2n-6)x^2 + (n^2-7n+12)x^4$.

Proof. The power of the indeterminate is the product of the degree of pair of vertices; from the proof of Lemma 2.14 we could see that there is a single edge in $\bar{P}_n$ which comprises of end vertices resulting into product of degree as 1, $(2n-6)$ edges comprising of pair of vertices of degrees 2 and 1 which leads to a product of their degrees as 2 and $\frac{n^2-7n+12}{2}$ edges which link vertices of degree 2 giving the product of each pair as 4. Noting that the coefficients of the indeterminate are the number of edges connecting vertices of respective degrees. □

2.4. Coindex Polynomials for Complete Graph K_n.

A complete graph K_n is of order n and size $\frac{n(n-1)}{2}$ [1].

Remark 2.16. All vertices of a complete graph are adjacent to each other, so $\forall \ v_i \in V(K_n)$ the $d(v_i) = (n-1)$ [3].

Lemma 2.17. *The Zagreb coindex of a complete graph is 0.*

Proof. It is obvious as $V(\bar{K}_n) = \emptyset$. □

2.5. Coindex Polynomials for a complete Bipartite Graph $K_{m,n}$.

A complete bipartite graph $K_{m,n}$ is a graph whose vertex set is partitioned into two. The order of a complete bipartite graph is given by $m+n$ and the size by mn [1].

Remark 2.18. The vertex set of a complete bipartite graph is partitioned into two sets say A and B with $|A| = m$ and $|B| = n$, so for $v_i \in A$ and $v_j \in B$ we have $d(v_i) = n$, $d(v_j) = m$ [10].

For the coindex Zagreb polynomials of a complete bipartite graph we need to look at how the complement of the graph will be.

Proposition 2.19. *The complement of a complete bipartite graph is a union of two complete graphs.*

Proof. Given a complete bipartite graph $K_{m,n}$ with partitions say A and B with $|A| = m$, $|B| = n$. Since the elements of partition A are not adjacent to each other, same vertices will now be adjacent in $\bar{K}_{m,n}$ leading to a complete graph K_m just as elements of B will lead to K_n. This implies that $\bar{K}_{m,n} = K_m \cup K_n$. □

Theorem 2.20. *The first coindex Zagreb polynomial for a complete bipartite graph is given by* $\frac{m(m-1)}{2}\ x^{2n} + \frac{n(n-1}{2}\ x^{2m}$.

Proof. The degree of vertex in partition A is n while that of a vertex in partition B is m as seen in Remark 2.18, the sum of degrees of adjacent vertices in the complement of $K_{m,n}$ will be $2n$ for vertices in K_m and $2m$ for vertices in K_n. Taking the sum over all the edges of the new graph has to do with edges of each complete graph separately. We now apply Equation 2.3

$$\bar{M}_1(K_{m,n}; x) = \sum_{uv \notin E(K_{m,n})} x^{[d_u\ +\ d_v]}$$

$$= x^{2n} \times |E|_{k_m} + x^{2m} \times |E|_{k_n} = \frac{m(m-1)}{2}\ x^{2n} + \frac{n(n-1)}{2} x^{2m}.$$

□

Note that if $m = n$, $\bar{M}_1(K_{m,n}; x) = m(m-1)x^{2m}$.

Theorem 2.21. *The second Zagreb coindex polynomial for a complete graph is given by* $\frac{m(m-1)}{2}\ x^{n^2} + \frac{n(n-1}{2}\ x^{m^2}$.

Proof. The proof is obtained in a similar way to that of Theorem 2.20 but with the product of degree of vertices as $d_u\ .\ d_v = n^2$ for vertices in partition A and $d_u\ .\ d_v = m^2$ for partition B. □

Note: if $m = n$, $\bar{M}_2(K_{m,n}; x) = m(m-1)x^{m^2}$.

3. Conclusion

In this paper we studied the compliment of special graphs like the cycle graph C_n, wheel W_n, path P_n, complete graph K_n and the complete bipartite graph $k_{m,n}$ and proposed a formula for computing the size of the compliment of a cycle graph ($|E(\bar{C}_n)|$) and path graph ($|E(\bar{P}_n)|$). For a complete bipartite graph it is shown that the compliment is a union of two complete graphs, formulae for obtaining the Zagreb coindex polynomials for the graphs under consideration are also given.

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